

Comparison of three different self-interaction corrections for an exactly solvable model system

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A systematic comparison of three approximate self-interaction corrections (SICs), Perdew-Zunger SIC, Lundin-Eriksson SIC and extended Fermi-Amaldi SIC, is performed for a model Hamiltonian whose exact many-body solution and exact local-density approximation (LDA) are known. For each of the three proposals we compare its implementation only for the potential, only for the energy (*i.e.*, a post-LDA evaluation of the SIC energy), to none of them (*i.e.*, a standard LDA calculation) and to both. Each of the resulting 10 permutations of methodologies is applied to 420 Hubbard chains differing in size, particle number and interaction strength. A statistical analysis of the resulting data set reveals trends and permits to assess the performance of each methodology. Overall, but not in each individual case, a post-LDA application of Perdew-Zunger SIC emerges as the recommended methodology.

I. INTRODUCTION

Density-functional theory (DFT)^{1,2,3} is advancing at a rapid pace, driven by the demand of ever more accurate electronic-structure calculations. To meet this demand, ever more sophisticated density functionals are being constructed. A simultaneous, and often contradictory, demand is the applicability to larger and more complex systems, met by computational and methodological advances in the implementation of density functionals. In this context, the comparison of different approximate density functionals and different modes of their implementation is of key importance. The present paper provides such a comparison for the case of self-interaction corrected functionals.

In Sec. II we recall three different self-interaction corrections. In Sec. III we discuss four different implementations, selected specifically to be able to compare the effect of self-interaction corrections on the potential and on the energy, in an unbiased way. In Sec. IV we report results from a statistical analysis of hundreds of calculations with each of the possible permutations of correction and implementation, for an exactly solvable model system whose exact many-body ground-state energy is known. Sec. V contains our conclusions.

II. SELF-INTERACTION ERROR AND SELF-INTERACTION CORRECTIONS

One electron does not interact with itself. Simple as it is, this fact is at the heart of much trouble in many-body and electronic-structure theory. Traditional density functionals, such as the local density, local spin-density and generalized-gradient approximations (GGAs), as well as many more recently developed functionals, such as hybrids and meta GGAs, do have a spurious self-interaction error (SIE), and as a consequence predict a nonzero in-

teraction energy even for a single electron. The *exact* exchange energy of one electron exactly cancels its Hartree energy, so that the Hartree + exchange energy of methods employing exact exchange is self-interaction free, but the correlation energy remains subject to self interaction even in methods employing exact exchange. Consequences of the SIE of approximate functionals are multifarious, and include wrong asymptotics of approximate exchange-correlation (*xc*) potentials, energy gaps, ionization energies, electron affinities and transition-metal magnetic moments.

Already in 1934, Fermi and Amaldi (FA)⁴ realized that Thomas-Fermi calculations, which use a local-density approximation for the noninteracting kinetic energy and approximate the full interaction energy by the Hartree energy,

$$E_H[n] = \frac{1}{2} \int d^3r \int d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (1)$$

suffer from a large SIE, and proposed a first self-interaction correction (SIC), of the form

$$E_H^{FASIC}[n] = \left(1 - \frac{1}{N}\right) E_H[n] = E_H[n] - \frac{1}{N} E_H[n]. \quad (2)$$

Equation (2) is clearly a very crude approximation, violating, among other things, the requirement of size-consistency, but it does eliminate the SIE of $E_H[n]$ for a one-electron system ($N = 1$).

After the development of modern density-functional theory, the question of how to eliminate the SIE posed itself anew. One way to carry over to modern Kohn-Sham DFT the simplicity of the FA approach is what we call extended-Fermi-Amaldi SIC (EFASIC), where the FA factor is applied not just to the Hartree energy, but to the sum of Hartree, exchange and correlation energies,

$$E_{xc}^{EFASIC}[n_\uparrow, n_\downarrow] = E_{xc}^{approx}[n_\uparrow, n_\downarrow] - \frac{1}{N} (E_H[n] + E_{xc}^{approx}[n_\uparrow, n_\downarrow]), \quad (3)$$

where $E_{xc}^{approx}[n_{\uparrow}, n_{\downarrow}]$ is an approximation, *e.g.* LDA or GGA, to the exact exchange-correlation functional.

A very successful proposal for a more sophisticated SIC, made in 1981 by Perdew and Zunger (PZ),⁵ is

$$E_{xc}^{PZSIC}[n_{\uparrow}, n_{\downarrow}] = E_{xc}^{approx}[n_{\uparrow}, n_{\downarrow}] - \sum_k \sum_{\sigma=\uparrow, \downarrow}^{occ} (E_H[n_{k\sigma}] + E_{xc}^{approx}[n_{k\sigma}, 0]), \quad (4)$$

where $n_{\sigma}(\mathbf{r}) = \sum_k^{occ} n_{k\sigma}(\mathbf{r})$, $n_{k\sigma}(\mathbf{r}) = |\varphi_{k\sigma}(\mathbf{r})|^2$, and $\varphi_{k\sigma}(\mathbf{r})$ are the Kohn-Sham (KS) orbitals.

In PZSIC, the SIE is subtracted on a orbital by orbital basis. Evidently, for a one-electron density $E_{xc}^{PZSIC}[n^{(1)}] = -E_H[n^{(1)}]$. The PZSIC functional depends on the orbitals $\varphi_{k\sigma}$, so that its minimization with respect to the density must employ the optimized-effective potential (OEP) method or one of its simplifications.^{6,7,8} In practice, however, the minimization is usually performed with respect to the orbital densities, and

$$\begin{aligned} v_{s,k\sigma}^{PZSIC}(\mathbf{r}) &= v_{ext}(\mathbf{r}) + v_H[n](\mathbf{r}) + v_{xc,\sigma}^{approx}[n_{\sigma}, n_{\bar{\sigma}}](\mathbf{r}) \\ &\quad - v_H[n_{k\sigma}](\mathbf{r}) - v_{xc,\sigma}^{approx}[n_{k\sigma}, 0](\mathbf{r}) \quad (5) \\ &=: v_{ext}(\mathbf{r}) + v_H[n](\mathbf{r}) + v_{xc,k\sigma}^{PZSIC}[n_{\sigma}, n_{\bar{\sigma}}](\mathbf{r}) \quad (6) \end{aligned}$$

is adopted as corresponding single-body potential. This potential is constructed from the density of *all* electrons.

The PZSIC approach, simplified by minimizing with respect to orbital densities instead of total densities, has been very succesful in removing the one-electron SIE in solids.⁹ Results from proper minimization with respect to the densities, by means of the OEP, are reported in, *e.g.*, Refs. 10,11 for atomic systems. PZSIC has become so popular that frequently the abbreviation SIC is used as synonymous with PZSIC, but it has been repeatedly noted that the PZ proposal is not the only possibility for removing the SIE.^{12,13,14,15}

An innovative proposal for an alternative self-interaction correction was put forward in 2001 by Lundin and Eriksson (LE).¹⁵ The LE proposal attempts to construct an effective potential that, when acting on the orbital of one electron, is constructed only from the density of the *other* electrons. In practice, this is done by introducing an orbital-dependent effective potential, $v_{s,k\sigma}(\mathbf{r})$, determined by subtracting from the full density $n(\mathbf{r})$ the partial density of the orbital the potential acts on,^{15,16}

$$\begin{aligned} v_{s,k\sigma}^{LESIC}(\mathbf{r}) &= v_{ext}(\mathbf{r}) + v_H[n - n_{k\sigma}](\mathbf{r}) \\ &\quad + v_{xc}^{approx}[n_{\sigma} - n_{k\sigma}, n_{\bar{\sigma}}](\mathbf{r}) \quad (7) \\ &= v_{ext}(\mathbf{r}) + v_H[n](\mathbf{r}) - v_H[n_{k\sigma}](\mathbf{r}) \\ &\quad + v_{xc}^{approx}[n_{\sigma} - n_{k\sigma}, n_{\bar{\sigma}}](\mathbf{r}) \quad (8) \\ &=: v_{ext}(\mathbf{r}) + v_H[n](\mathbf{r}) + v_{xc,k\sigma}^{LESIC}[n_{\sigma}, n_{\bar{\sigma}}](\mathbf{r}). \quad (9) \end{aligned}$$

In this way, the approximate effective potential acting on a given orbital, $v_{s,k\sigma}^{LESIC}(\mathbf{r})$, is constructed only from the density arising from the other orbitals. Clearly, for

a one-particle system this approach also correctly zeroes the interaction contribution to the effective potential.

The LE proposal for a corrected effective potential is accompanied by a similar expression for the exchange-correlation energy,^{15,17}

$$\begin{aligned} E_{xc}^{LESIC}[n_{\uparrow}, n_{\downarrow}] &= - \sum_k \sum_{\sigma=\uparrow, \downarrow}^{occ} E_H[n_{k\sigma}] \\ &\quad + \sum_k \sum_{\sigma=\uparrow, \downarrow}^{occ} \int d\mathbf{r}^3 n_{k\sigma}(\mathbf{r}) e_{xc}^{approx}[n_{\sigma} - n_{k\sigma}, n_{\bar{\sigma}}]. \quad (10) \end{aligned}$$

We note that the change from the LESIC to the PZSIC approach can be affected by substituting

$$e_{xc}^{approx}[n_{\sigma} - n_{k\sigma}, n_{\bar{\sigma}}] \rightarrow e_{xc}^{approx}[n_{\sigma}, n_{\bar{\sigma}}] - e_{xc}^{approx}[n_{k\sigma}, 0] \quad (11)$$

and

$$v_{xc}^{approx}[n_{\sigma} - n_{k\sigma}, n_{\bar{\sigma}}] \rightarrow v_{xc,\sigma}^{approx}[n_{\sigma}, n_{\bar{\sigma}}] - v_{xc,\sigma}^{approx}[n_{k\sigma}, 0] \quad (12)$$

in the xc energy density and potential of former. For the Hartree potential, the substitution $v_H[n - n_{k\sigma}] \rightarrow v_H[n] - v_H[n_{k\sigma}]$ is an identity.

The LE energy expression (10) is constructed in analogy to Eq. (9), but its functional derivative is not the LE xc potential in Eq. (9). Rather, both are separate constructions. This gives rise to a certain ambiguity in how to implement the LE approach. Sec. III we therefore discuss various alternative implementations of Eqs. (9) and (10).

In the original LE work¹⁵ it was argued that the LE approach should be superior to the PZ approach because it removes the SIE of the potential, which, according to Ref. 15, remains in the PZ approach. It has been objected¹⁸ that the LE proposal cannot be right because it would even correct the hypothetical exact functional, for which the PZ approach correctly reduces to zero.

While we agree with this objection as a matter of principle, we feel that in practice the key issue is not only what the correction does to the hypothetical exact functional, but also what it does to actually available approximate functionals. If such functionals were consistently improved by a correction, few workers would refrain from using this correction in practice, only because it overcorrects the hypothetical exact functional.

Interestingly, there are hints in the literature that approximate xc functionals do indeed benefit more from LESIC than from PZSIC. Novak et al.¹⁶ compare the performance of LSDA, LSDA+PZSIC and LSDA+LESIC in the calculation of hyperfine parameters, and find that LESIC significantly improves agreement with experiment, relative to PZSIC. (See also Ref. 19 for a successful application of LESIC to hyperfine parameters.) In a separate study, Friis et al.²⁰ compared density distributions predicted for the Mg crystal with experimental electron diffraction data, and observed that LESIC produces better core and valence densities than PZSIC.

The available data are too limited, however, to already conclude that LESIC is definitely superior, in practice, to PZSIC, in particular since, as a matter of principle, LESIC cannot be correct. It therefore becomes an important task to systematically investigate the performance of both approaches. The present paper is a first step towards this task, providing a systematic analysis of the performance of PZSIC, LESIC and EFASIC for a well controlled model system whose exact solution is known.

III. IMPLEMENTATION

Formally, the xc potential corresponding to a given approximation to $E_{xc}[n_\sigma, n_{\bar{\sigma}}]$ is

$$v_{xc,\sigma}^{approx}[n_\sigma, n_{\bar{\sigma}}](\mathbf{r}) = \frac{\delta E_{xc}^{approx}[n_\sigma, n_{\bar{\sigma}}]}{\delta n_\sigma(\mathbf{r})}. \quad (13)$$

We have just seen, however, that by construction the LE xc potential is not the derivative of the LE xc energy, but a separate construction. Strictly speaking, the same is true for most common implementations of PZSIC, where the implemented potential is the orbital derivative, and not the density derivative of the energy. This ambiguity suggests that a complete test of each proposal involves four different permutations of methodologies.

Our notation for these is APPV-APPE, where APPV represents the approximation made for the potential entering the KS equations, and APPE the approximation made for the energy functional. The simplest possibility is thus LDA-LDA, which is a standard LDA calculation using the L(S)DA potential and energy.²¹ The second scheme, denoted LDA-SIC, consists of a self-consistent LDA calculation, followed by a single evaluation of the SIE corrected energy functional on the LDA densities and orbitals. This strategy is also known as post-LDA implementation of SIC. By construction, it tests the performance of the SIC for the xc energy. The inverse possibility, which we label SIC-LDA, is a self-consistent SIC calculation, followed by a single evaluation of the uncorrected LDA energy functional on the corrected densities. This procedure tests the performance of the employed xc correction for the potentials. Finally, SIC-SIC refers to a calculation using the SIC under study both in the potential and the energy. Starting from LDA-LDA, each of the other three possibilities can be implemented for each of the three SICs described in the previous section, resulting in a total of ten combinations of methodologies.

In the self-consistent implementation of the PZSIC potential obtained from the orbital derivative of the PZ energy and of the LESIC potential, which are required in schemes SIC-LDA and SIC-SIC, we face the additional difficulty that these potentials are not common multiplicative potentials for all KS orbitals, but are orbital-specific, *i.e.* different for each orbital they act on. Such orbital-specific potentials, $v_k[\{\varphi_j[n]\}](\mathbf{r})$, are not proper Kohn-Sham potentials, although they are still density functionals.

A common multiplicative potential for all orbitals can be generated from the PZ and LE energy functionals by means of the OEP, but in the case of LESIC the potential resulting from the energy functional (10) would have no relation to the LE potential (9), which, as we have seen above, is a separate construction. Hence, implementation via the OEP would implicitly test the proposed energy correction (10), not the proposed potential correction (9), required in the schemes SIC-LDA and SIC-SIC.

A way to directly compare the orbital-specific PZ and LE potentials is to average the xc potentials over all orbitals, weighted with the contribution each orbital makes to the full spin density, according to²²

$$\bar{v}_{xc,\sigma}^{PZSIC}[n_\sigma, n_{\bar{\sigma}}](\mathbf{r}) = v_{xc,\sigma}^{approx}[n_\sigma, n_{\bar{\sigma}}](\mathbf{r}) - \sum_k^{occ} (v_H[n_{k\sigma}](\mathbf{r}) + v_{xc}^{approx}[n_{k\sigma}, 0](\mathbf{r})) \frac{n_{k\sigma}(\mathbf{r})}{n_\sigma(\mathbf{r})} \quad (14)$$

and

$$\bar{v}_{xc,\sigma}^{LESIC}[n_\sigma, n_{\bar{\sigma}}](\mathbf{r}) = - \sum_k^{occ} (v_H[n_{k\sigma}](\mathbf{r}) - v_{xc}^{approx}[n_\sigma - n_{k\sigma}, n_{\bar{\sigma}}](\mathbf{r})) \frac{n_{k\sigma}(\mathbf{r})}{n_\sigma(\mathbf{r})} \quad (15)$$

The result are average multiplicative potentials arising from the orbital-specific LE or PZ potential. Of course, some information is lost in the averaging, but since our aim is to compare LE and PZ among each other, the errors of the averaging procedure are of secondary importance, as long as all functionals are treated in the same way.

We note that in the case of the PZ correction the same averaged potential is also obtained by applying the OEP algorithm to the PZ xc functional, which in the first step leads to

$$v_{xc,\sigma}^{PZSIC}[n_\sigma, n_{\bar{\sigma}}](\mathbf{r}) = \frac{\delta E_{xc}^{PZSIC}[n_\sigma, n_{\bar{\sigma}}]}{\delta n_\sigma(\mathbf{r})} \quad (16)$$

$$= v_{xc,\sigma}^{approx}[n_\sigma, n_{\bar{\sigma}}](\mathbf{r}) - \sum_{k\tau}^{occ} \int d^3r' (v_H[n_{k\tau}](\mathbf{r}) + v_{xc}^{approx}[n_{k\tau}, 0](\mathbf{r})) \frac{\delta n_{k\tau}(\mathbf{r}')}{\delta n_\sigma(\mathbf{r})} \quad (17)$$

and then making the Slater approximation²²

$$\frac{\delta n_{k\tau}(\mathbf{r}')}{\delta n_\sigma(\mathbf{r})} \approx \frac{n_{k\tau}(\mathbf{r}')}{n_\sigma(\mathbf{r})} \delta(\mathbf{r} - \mathbf{r}') \delta_{\sigma\tau} \quad (18)$$

for the functional derivative. In this sense, our SIC-LDA and SIC-SIC implementations of PZSIC are approximate OEP calculations. As explained above, the same is not true for LESIC, where the OEP would produce the local xc potential coming from the LE xc energy (10), which is not the same as the LE xc potential in Eq. (9) or its average (15). In the present context, it is the averaging prescription which must be employed to test the LE proposal for the potential, not the OEP.

Finally, the question poses itself by what standard we are to measure the performance of a SIC. Comparison to experiment is hard because the SIE itself is not an experimental observable, and analysis of fine differences between computational approaches relative to experiment is complicated by effects such as relativity, finite temperature, zero-point vibrations, sample purity, etc. that are of no direct relevance to the calculation, but automatically included in the experimental value. Even on the purely computational side, the issue is thorny, because the approximate SIC is applied to a functional, such as LDA, that is itself approximate, and it is not always easy to disentangle the error of the functional from that of its correction, or from that of approximations such as the sphericalization of atomic densities often used in PZSIC calculations. Moreover, calculations for real systems involve basis sets or numerical meshes, whose adequateness must be carefully tested, and which may introduce further residual uncertainties in the calculations.

For all these reasons, we perform our analysis using as theoretical laboratory a very well controlled model Hamiltonian: the one-dimensional Hubbard model

$$\hat{H} = -t \sum_{i,\sigma}^L \left(c_{i\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.} \right) + U \sum_i^L c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}. \quad (19)$$

This model, which may be considered a special case of the PPP model popular in quantum chemistry,²³ describes electrons on a one-dimensional lattice of size L , interacting with on-site interaction U , and hopping from one site i to the next with amplitude t . Occupation of each site is limited to two particles, necessarily of opposite spin. Like-spin particles do not interact in the most common form of the model. The basic Hohenberg-Kohn and Kohn-Sham theorems of DFT hold for this model, too, once the density $n(\mathbf{r})$ is replaced by the on-site occupation number^{24,25}

$$n(\mathbf{r}) = \sum_{\sigma} n_{\sigma}(\mathbf{r}) \rightarrow n_i = \sum_{\sigma} n_{i\sigma} = \sum_{\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle. \quad (20)$$

In terms of this variable, local-density and spin-density approximations for Hubbard chains and rings have been constructed,^{26,27,28,29} and can be employed in the usual way.

What makes this model attractive as a theoretical laboratory for DFT is that its exact many-body solution is known in the thermodynamic limit ($L \rightarrow \infty$, $n_i = n = \text{const}$),³⁰ and an exact numerical solution is possible for small systems ($L \sim 14$ on a workstation, for arbitrary density distributions n_i). As a consequence of the availability of the exact solution for the infinite homogeneous system, the exact LDA is known, too.³¹ Moreover, a complete basis consists of two spin-orbitals per site, so that we can always work at the basis-set limit. Another welcome feature, which we will exploit below, is that the model allows to continuously vary the interaction strength both in the exact and in the DFT calculations, which simulates the behavior of weakly and strongly interacting systems in *ab initio* calculations.

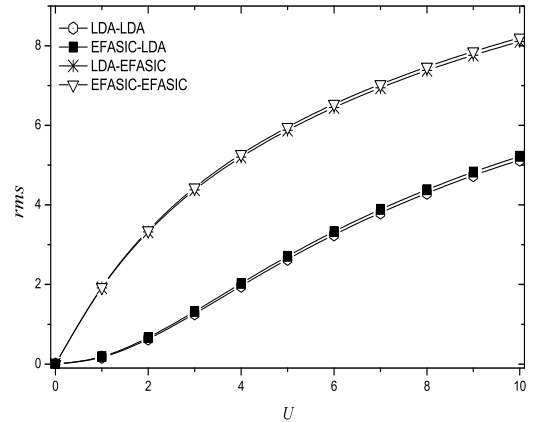


FIG. 1: Root-mean-square error, in percent, of the different implementations of the Extended Fermi-Amaldi self-interaction correction (EFASIC), relative to the exact many-body ground-state energy. $N_s = 42$ systems are considered at each U/t .

IV. RESULTS

In this section we compare the three self-interaction corrections EFASIC, LESIC and PZSIC, in the LDA-LDA, LDA-SIC, SIC-LDA and SIC-SIC schemes, using the orbital (Slater-type) average of Eqs. (14) and (15) to deal with the orbital-specific PZ and LE potentials in the schemes SIC-LDA and SIC-SIC. All calculations are done for finite chains of different lengths L , particle numbers N and interaction strengths U . Variation of these parameters for each combination of methodology produces thousands of data, which we analyze statistically by reporting the percentage root-mean-square (rms) error,

$$rms = 100 \sqrt{\frac{1}{N_s} \sum_{j=1}^{N_s} \left(\frac{E_{approx}^j - E_{exact}^j}{E_{exact}^j} \right)^2}, \quad (21)$$

of each approximation relative to numerically exact many-body energies for the same set of model parameters. N_s is the number of systems in the data set, labelled by j .

Our results are summarized in Figs. 1 to 3 and in Table I. Each of the three figures compares the rms error defined in Eq. (21) as a function of interaction strength U , ranging from the noninteracting system $U = 0$, over weakly $U \sim 2t$, strongly $U \sim 6t$ to very strongly, $U \sim 10t$, interacting systems. For each value of U/t , our sample consists of $N_s = 42$ systems of different sizes, particle number, and densities ($L = 3, 4, 5..14$ and $N = 2, 4, 6, ..12$, with $N/L < 1$).

We can analyze these figures from two different points of view. First, comparing the three corrections, we find that PZSIC consistently performs much better than

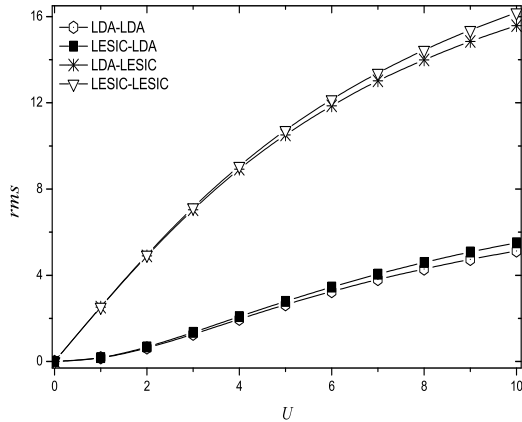


FIG. 2: Root-mean-square error, in percent, of the different implementations of the Lundin-Eriksson self-interaction correction (LESIC), relative to the exact many-body ground-state energy. $N_s = 42$ systems are considered at each U/t .

LESIC or EFASIC. The scale on the vertical axis of the three figures is not the same, to permit a better visualization of the differences between the various implementation schemes, but the values of the rms error are directly comparable, and leave little doubt about the superiority of PZSIC for these systems. Somewhat surprisingly, the very simple EFASIC still performs a little better than the more sophisticated LESIC. Of course, our conclusions are based only on ground-state energies, but since the difference in performance for the energy is quite large, and since many other observables are obtained from energies, we expect that PZSIC should be superior to the others in most applications.

Second, comparing modes of implementation, we find that they fall in two groups, distinguished by the energy functional: The schemes LDA-LDA and SIC-LDA always give similar results, as do the schemes LDA-SIC and SIC-SIC. The two schemes in the first group evaluate the LDA energy functional on self-consistent (LDA or SIC) densities, while the two schemes in the second group evaluate the SIC energy functional on self-consistent (LDA or SIC) densities. The formation of these two groups, occurring in the same manner for each of the three corrections, shows us that what matters for the final result is the energy functional evaluated once on selfconsistent densities, not the potential employed during the iterations to self-consistency. This observation gives support to common post-LDA implementations of complex functionals.

For EFASIC and LESIC, the implementations in group two perform much worse than those in group one. Within group one, SIC-LDA does slightly worse than LDA-LDA, while within group two SIC-SIC is slightly worse than LDA-SIC. For all U/t , a simple selfconsistent LDA calculation is better than a calculation employing EFASIC or LESIC for the potential, the energy, or both.

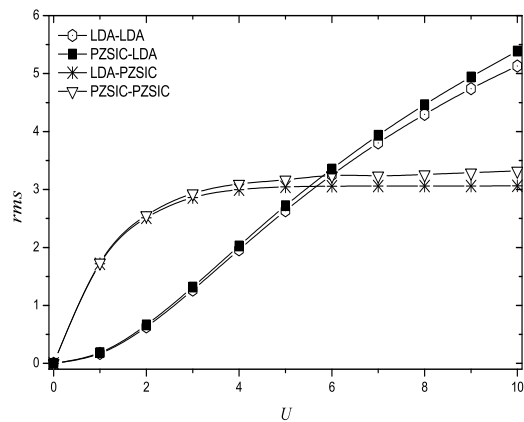


FIG. 3: Root-mean-square error, in percent, of the different implementations of the Perdew-Zunger self-interaction correction (PZSIC), relative to the exact many-body ground-state energy. $N_s = 42$ systems are considered at each U/t .

For PZSIC, a crossover between the error curves occurs around $U \sim 5t$. Below this value, the picture is the same, qualitatively, as for LESIC and EFASIC: it is better to do a simple LDA calculation than to apply PZSIC in any implementation. Above $U \sim 5t$, the situation changes, and the schemes in group two (LDA-PZSIC and PZSIC-PZSIC) perform clearly better than those in group one.³² Hence, only PZSIC is a real improvement on the LDA, and this improvement manifests itself only for sufficiently strongly interacting systems.

As the data show, for weakly interacting systems (where the physics is dominated by the kinetic energy term, and the particles are delocalized) LDA is still better than PZSIC. Of course, PZSIC removes the self-interaction error of the LDA also in this regime, but PZSIC itself is not exact, and thus introduces other errors. For weak interactions, it does not pay to correct a small error by a correction introducing larger ones. For stronger interactions, the particles start to localize, the SIE becomes more important, and its removal by PZSIC improves the total energies considerably. The separation in these two regimes is a very gratifying result to obtain, as $U \sim 5t$ is known to mark the region where the Hubbard model crosses over from weakly to strongly interacting systems, and the electrons become increasingly localized. The performance of PZSIC is clearly correlated with this crossover. In fact, in retrospect, one could have predicted that the electrons in the Hubbard model start to localize around $U \approx 5t$ simply by comparing the relative performance of LDA and LDA+PZSIC as a function of U/t .

To make this division in two distinct regimes clearer, we report in Table I the rms error for each regime, *i.e.*, sum not only over systems with different size and particle number, but also over those with interaction strengths

TABLE I: Root-mean-square error for all weakly and all strongly interacting systems (columns 1 and 2) and for all investigated systems (column 3), for all ten permutations of methodologies investigated here. Entries in boldface are the best in each column (interaction regime).

Method	$U/t = 1..5$	$U/t = 6..10$	$U/t = 1..10$
N_S	210	210	420
LDA-LDA	1.6008	4.2957	3.2416
LDA-EFASIC	4.3713	7.3541	6.0494
EFASIC-EFASIC	4.4266	7.4423	6.1230
EFASIC-LDA	1.6551	4.3827	3.3126
LDA-PZSIC	2.6724	3.0596	2.8726
PZSIC-PZSIC	2.7471	3.2693	3.0189
PZSIC-LDA	1.6567	4.4749	3.3741
LDA-LESIC	7.3476	13.9210	11.1306
LESIC-LESIC	7.4749	14.3770	11.4580
LESIC-LDA	1.7020	4.5960	3.4655

in the indicated range. The lowest rms error in each regime is printed in boldface. Clearly, for weakly interacting systems, LDA-LDA does best, but PZSIC-LDA and EFASIC-LDA are only marginally inferior because the SIC chosen for the potential does not matter much, compared to the effect of the energy functional. For strongly interacting systems, on the other hand, LDA-PZSIC wins, closely followed by PZSIC-PZSIC. Overall, *i.e.* considering the rms error over all considered systems, regardless of the value of U/t , LDA-PZSIC is the best combination of correction and implementation among all methodologies tested here.

We finally remark that the peculiar aspect of the LE approach, where the SIC potential is neither the density derivative nor the orbital derivative of the SIC energy, but a separate construction, does not seem to cause any additional features in the results. As we found above, the effect of the potential of any SIC is much less important than that of its energy, so the inconsistency between them in the LE approach apparently does not matter much.

V. CONCLUSIONS

We compared selfconsistent LDA calculations, three self-interaction corrections applied to the LDA, and three ways to implement each correction, for a total of 420 systems, for each of which we also obtained, numerically, the exact many-body solution. Three clear trends emerge from the resulting 4200 approximate and 420 exact data: (i) For all three investigated corrections, the main effect comes from the energy, not the potential. Post-LDA implementations (correcting only the energy) and selfconsistent implementations (correcting the energy and the potential) give very similar results,³² while implementing only the correction to the potential has virtually no effect on the resulting ground-state energies. (ii) For weakly interacting systems, the benefit of an approximate SIC is overcompensated by the intrinsic errors of the approximation. Uncorrected LDA here works best. (iii) For more strongly interacting systems, correcting the SIE is important, but of the three investigated corrections only PZSIC systematically improves on the LDA. Both the simple EFASIC and the more sophisticated LESIC are much worse.

Of course, all our conclusions may have been biased by the choice of the Hubbard model as theoretical laboratory. The disadvantages of such possible bias, on the other hand, are largely compensated by the availability of an exact many-body solution as a benchmark, of the exact LDA,³¹ and by the absence of any problems due to finite basis sets or due to experimental uncertainties. It remains to be seen if the superiority of PZSIC remains unchallenged by extension of these investigations to other corrections, implementations and classes of systems. Similarly, the important issue of the many-electron SIE^{33,34} requires separate investigation.

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